Chaotic Electron Motion in Superlattices. Quantum-Classical Correspondence of the Structure of Eigenstates and LDOS.

G. A. Luna-Acosta, J. A. Méndez-Bermúdez, and F. M. Izrailev

Instituto de Física, Universidad Autónoma de Puebla, Puebla, Pue. 72570, Apartado Postal J - 48, México.

Abstract

We investigate the classical-quantum correspondence for particle motion in a superlattice in the form of a 2D channel with periodic modulated boundaries. Its classical dynamics undergoes the generic transition to chaos of Hamiltonian systems as the amplitude of the modulation is increased. We show that for strong chaotic motion, the classical counterpart of the structure of eigenstates (SES) in energy space reveals an excellent agreement with the quantum one. This correspondence allows us to understand important features of the SES in terms of classical trajectories. We also show that for typical 2D modulated waveguides there exist, at any energy range, extremely localized eigenstates (in energy) which are practically unperturbed by the modulation. These states contribute to the strong fluctuations around the classical SES. The approach to the classical limit is discussed.

PACS: 05.45+b, 03.20.

A variety of important physical systems are periodic, either in space; such as crystals and superlattices; in time, like periodically forced mechanical devices; or in both, as in particle motion in a superlattice subject to an ac electric field. The analysis of such systems has lead to the understading of well known fundamental phenomena, e.g., energy band structure of solids and resonances. On the other hand, during the last decade much attention have been paid to to study the classical-quantum correspondence (CQC) of classically chaotic systems. In [1] we give references to some interesting physical time-periodic chaotic systems. One of the challenges is to identify the ways in which classical chaos may be manifested in the quantum regime [2]. There are well established tools to characterize a quantum classically chaotic system. The most commonly used relies on the analysis of their spectra (e.g., level spacing distribution) in the context of the random matrix theory conjecture [3]. See also [4] for other signatures of "quantum chaos".

Here we explore the CQC of the particle motion in a superlattice in the form of a 2D electron waveguide with periodically modulated boundaries. Two possible experimental realizations are: 1) a film whose thickness is a periodic function of one of the coordinates and 2) a periodically modulated mesoscopic electron channel in the ballistic regime (see [5,6] and references therein). We analyze the problem by studying the structure of the eigenfunctions (SEF) and local density of states (LDOS) [7]. This novel approach has been applied recently to a variety of systems [8]. The basic idea is as follows. Consider a non-integrable Hamiltonian $H = H_0 + V$, where V is the non-integral perturbation to the integrable Hamiltonian H_0. Let the eigenstates of H and H_0 be denoted, respectively, by Ψ^α and ϕ_j. We can then form the matrix $w_l^\alpha \equiv |C_l^\alpha(k)|^2$, where $C^\alpha_j =< \Psi^\alpha \mid \phi_j >$. The rows (columns) of w_l^α show how a specific perturbed eigenstate $|\alpha >$ (unperturbed eigenstate $\phi >$) is expanded in the unperturbed basis $|l >$ (perturbed basis $\alpha >$). For our purposes it is essential, as will become clear below,

to energy-order the unperturbed as well as the perturbed states; that is, $E^{\alpha+1} \geq E^{\alpha}$ and $E^0_{l+1} \geq E^0_l$, where E^{α} and E^0_l are the energy spectra of the perturbed and unperturbed systems, respectively; $\alpha, l = 1, 2....$ The structure of eigenstastes SES is defined as [7],

$$W(E^0_l \mid E^{\alpha}) = \sum_{\alpha'} \bar{w}^{\alpha'}_l \, \delta(E^0_l - E^{\alpha'}), \qquad (1)$$

where $\bar{w}^{\alpha'}_l = w^{\alpha'}_l / N$ with N as the number of eigenstates $|\alpha' >$ in the vicinity of a given α. Eq. (1), seen as a function of the unperturbed energy E^0_l gives the structure of eigenstates with total energy close to E^{α}. The local density of states LDOS, also known as the strength function, defined as $\omega(E^{\alpha} \mid E^0_l) = \sum_{l'} \bar{w}^{\alpha}_{l'} \, \delta(E^{\alpha} - E^0_{l'})$, is also used to study the quantum-classical correspondence [6,8,9]. Here, for lack of space we shall not discuss it.

Now, the reason these two quantities, SES and LDOS, help us tackle the quantum-classical correspondence is that they have well defined classical counterparts [7]. Since $C^{\alpha}_l =< \Psi^{\alpha} \mid \phi_l >$ as a function of l is the *projection* of the perturbed state onto the states of the unperturbed system, the classical counterpart of $w^{\alpha}_l =\mid C^{\alpha}_l \mid^2$ as a function of energy E_l can be defined as the *projection* of the total Hamiltonian H onto the unperturbed one H^0, where $H = H^0 + V$ with V the perturbation. This can be numerically done by substituting the trajectories $\Phi(t) \equiv (x(t), y(t), p_x(t), p_y(t))$ generated by H with energy E into H^0. Since the unperturbed energy $E^0(t)$ along these trajectories varies in time, it fills the so-called *energy shell* characterized by its width ΔE. For chaotic total Hamiltonians H, the classical analog $W_{cl}(E^0 \mid E)$ of the quantum SES is the probability distribution constructed from $E^0(t)$. See below for details.

Similarly, the classical analog of LDOS can be obtained by performing the inverse operation, namely, projecting the dynamics of H^0 onto the Hamiltonian function H.

This approach assumes that the Hamiltonian could be separated into unperturbed and perturbed parts. For billiards, like our system, the non-integrability comes from the boundary conditions; the Hamiltonian operator, being simply the kinetic energy, is the same for both perturbed (periodically modulated) and unperturbed (flat) channel. To overcome this problem, a transformation to curvilinear coordinates can be performed such that both, perturbed and unperturbed systems have the same boundary conditions. Consequently the effects of the boundary appear in the new coordinates as an interaction potential between the two degrees of freedom (see details in [9]).

Since the Hamiltonian is periodic, the energy eigenstates satisfy Bloch's theorem. Although most of the results will be independent of the details of the profile, we need to specify a particular one. As in [5,6,9] we define the top boundary by $y = d + a\cos(x)$ and the bottom boundary by $y = 0$. The first classical dynamical studies of this system appear in [10,11]. The finite length version this system was analyzed in [12] as a model of a mesoscopic electron waveguide, where a transport signature of chaos in the behavior of resistivity was established. Ketzmerick [13] also used it to study certain *quantum* transport properties through ballistic cavities. Moreover, the analysis of the band-energy spectrum for an *infinitely* long rippled channel [5] in the cases of mixed and global classical chaos, yields insight into the universal features of electronic band structures of real crystals [14]. See also [15]. Results obtained for this particular system are applicable to a large class of systems, namely non-degenerate, non-integrable Hamiltonians. We limit this report to the case of global classical chaos which occurs in wide ($d > 2\pi$) channels [5]. The geometrical parameters used here are $(a/2\pi, d/2\pi) = (0.12, 0.5)$. Fig. 1 shows the unperturbed energy $E^0(t)$ obtained as explained above. The distribu-

tion of energies on the right of Fig. 1 is, by definition, the classical counterpart of SES, obtained by averaging $E^0(t)$ over time.

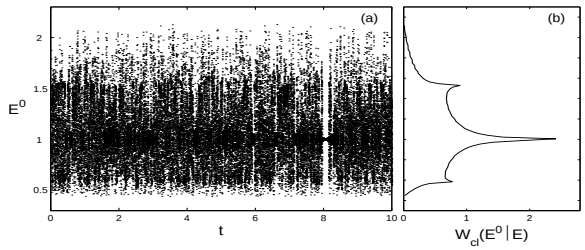

FIG. 1 a) $E^0(t)$ as a function of time (in arbitrary units) for $E = 1$. b) Classical SES $W_{cl}(E^0 \mid E)$.

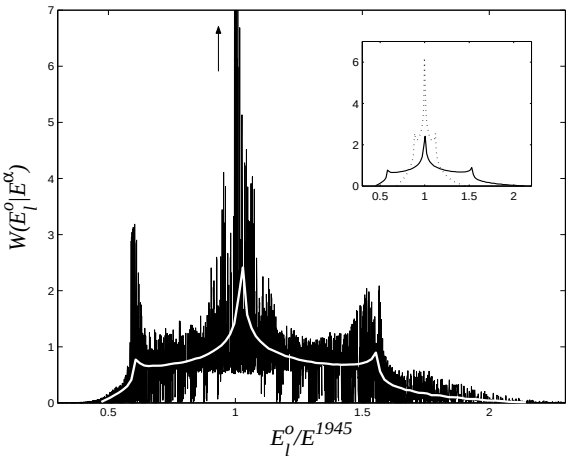

FIG. 2 Structure of eigenstates. Quantum SES (black line); Classical SES (white line). The average for the SES is over $1900 < \alpha < 1990$. Inset: classical SES for $(a/2\pi, d/2\pi) = (0.06, 1)$ (dotted) and $(a/2\pi, d/2\pi) = (0.12, 0.5)$ (continuous).

Fig. 2 compares the quantum and classical SES. We see that the classical SES agrees well with the average shape of quantum SES. *I.e.*, the classical SES predicts: 1) the appearance of three prominent peaks at specified values, 2) the width of the distribution (the energy shell); and 3) its assymmetry about 1. The inset compares classical SES for two channels defined by different geometrical parameters but both displaying global chaos in phase space. Thus, the classical and quantum SES can detect *dynamical differences not revealed by the standard tools*, e.g., Poincarè maps, and thus serves to complement the characterization of dynamical systems. In fact, detailed analysis [9] demonstrates that the left (right) side peak is formed by trajectories dwelling near the unstable (stable) fixed period-one fixed point, whereas the central peak is due to grazing trajectories.

The strong fluctuations of the quantum SES are due to: 1) the fact that the system is still not deep in the semiclassical regime (although the level numbers are high) and 2) the existence of extremely localized and sparse (in energy space) states. See below and [9] for details.

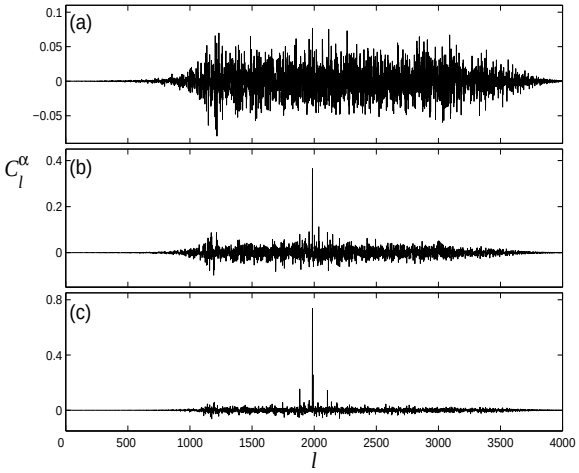

FIG. 3 Typical eigenfunctions. a) α=1984, b) α=1985, and c) α=1986.

Fig. 3 shows 3 consecutive eigenstates in the energy-ordered unperturbed basis, illustrating the kind of eigenstates that can occur typically: extended, sparse, and localized in the energy representation. A quantitative characterization is given by various localization measures, such as the entropy localization length l_H, the inverse participation ratio l_{ipr}, and the mean square root l_σ. See [6] for their definitions. In Fig. 4 we present l_H as a function of the perturbed state. It shows wild fluctuations, due to the existence of the localized and sparse states mentioned above. The extremely localized states are those that are practically the same as the unperturbed

(flat channel) states with transversal mode number $m = 1$. It can be shown that the number of these states $N_{m=1}$, relative to the total number of states $N(E)$, up to energy E, is given by $N_{m=1}/N(E) = 4/\pi\sqrt{E}$.

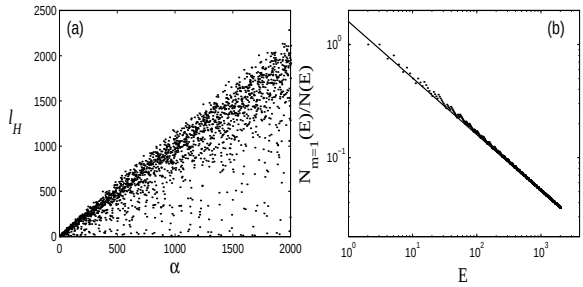

FIG. 4 (a) Entropy localization length l_H as a function of α. (b) $N_{m=1}(E)/N(E)$ as a function of E (dots) for the first 2000 states. The solid line is the analytical estimate $4/\pi\sqrt{E}$.

The fact that $N_{m=1}/N(E)$ decays as $1/\sqrt{E}$ implies that in the strict classical limit the fluctuations, observed in Fig. 2 for the quantum SES, will vanish, however, the approach to this limit is surprisingly slow. Furthermore, it can be shown that $N_{m=1} = 2\pi\sqrt{E}/d$, where d is the width of the channel, in units of the period of the ripple. This indicates that localized states continue to appear at all energies, even in the classical limit!. That is, one can always find states that remain practically unperturbed by the modulation. The importance of these extremely localized states in finite electron waveguides with modulated or corrugated boundaries is addressed in [16].

Acknowledgements. We acknowledge support by CONACyT grant, No. 26163-E, and NSF-CONACyT, grant No. E120-3341.

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